

ring nodes :

2 3 4 6 7 8 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33

ring/chain nodes :

1 5 9 10 11 12 13 14 15

ring/chain bonds :

1-2 1-9 1-10 4-5 5-11 5-12 6-13 10-15 13-14 15-22 15-31

ring bonds :

2-3 2-8 3-4 4-6 6-7 7-8 16-17 16-20 17-18 18-19 19-20 19-21 20-24 21-22
22-23 23-24 25-26 25-29 26-27 27-28 28-29 28-30 29-33 30-31 31-32 32-33

exact/norm bonds :

1-2 4-5 15-22 15-31

exact bonds :

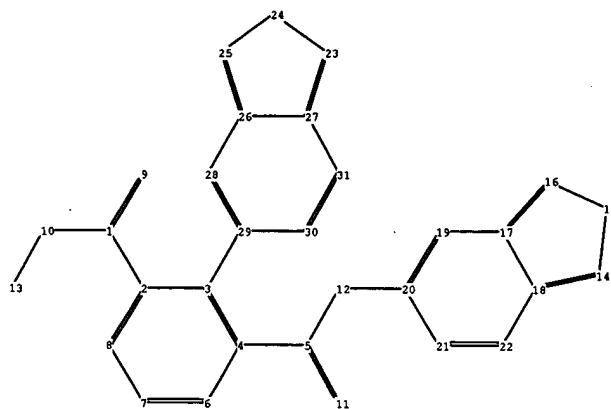
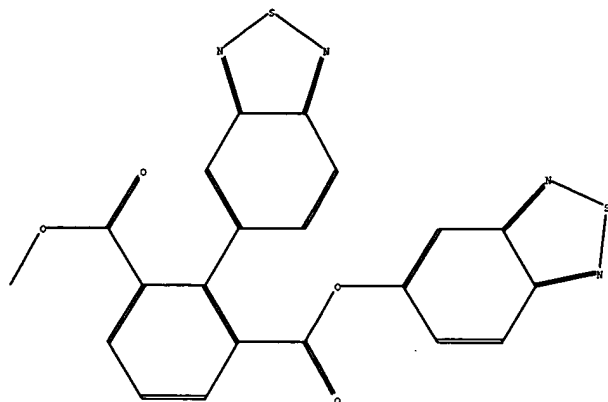
1-9 1-10 5-11 5-12 6-13 10-15 13-14 16-17 16-20 17-18 18-19 19-20 19-21
20-24 21-22 22-23 23-24 25-26 25-29 26-27 27-28 28-29 28-30 29-33 30-31 31-32
32-33

normalized bonds :

2-3 2-8 3-4 4-6 6-7 7-8

Match level :

1:CLASS 2:Atom 3:Atom 4:Atom 5:CLASS 6:Atom 7:Atom 8:Atom 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom
30:Atom 31:Atom 32:Atom 33:Atom



ring nodes :

2 3 4 6 7 8 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31

ring/chain nodes :

1 5 9 10 11 12 13

ring/chain bonds :

1-2 1-9 1-10 3-29 4-5 5-11 5-12 10-13 12-20

ring bonds :

2-3 2-8 3-4 4-6 6-7 7-8 14-15 14-18 15-16 16-17 17-18 17-19 18-22 19-20
20-21 21-22 23-24 23-27 24-25 25-26 26-27 26-28 27-31 28-29 29-30 30-31

exact/norm bonds :

1-2 3-29 4-5

exact bonds :

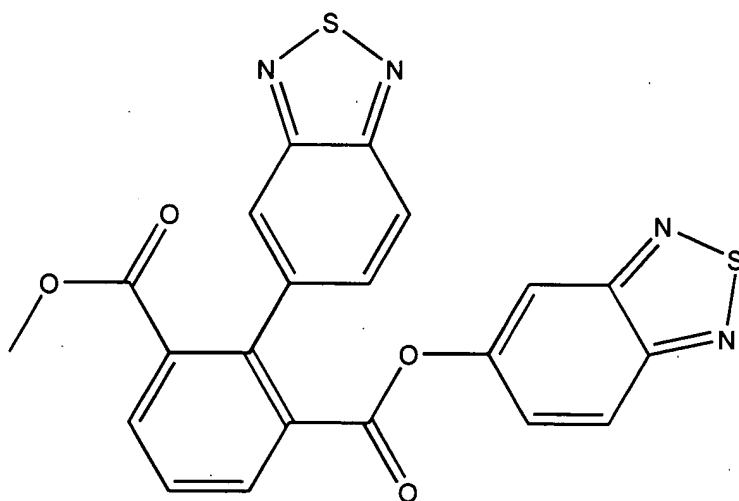
1-9 1-10 5-11 5-12 10-13 12-20 14-15 14-18 15-16 16-17 17-18 17-19 18-22
19-20 20-21 21-22 23-24 23-27 24-25 25-26 26-27 26-28 27-31 28-29 29-30 30-31

normalized bonds :

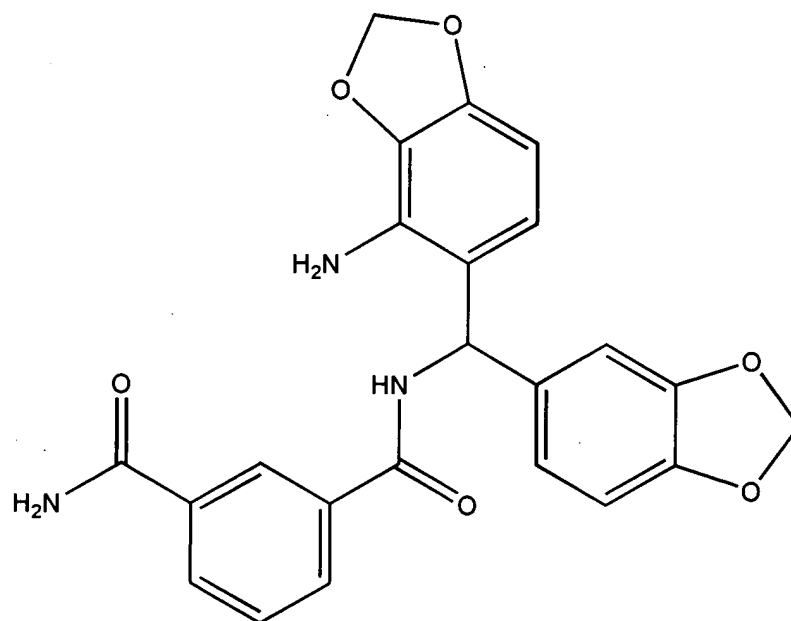
2-3 2-8 3-4 4-6 6-7 7-8

Match level :

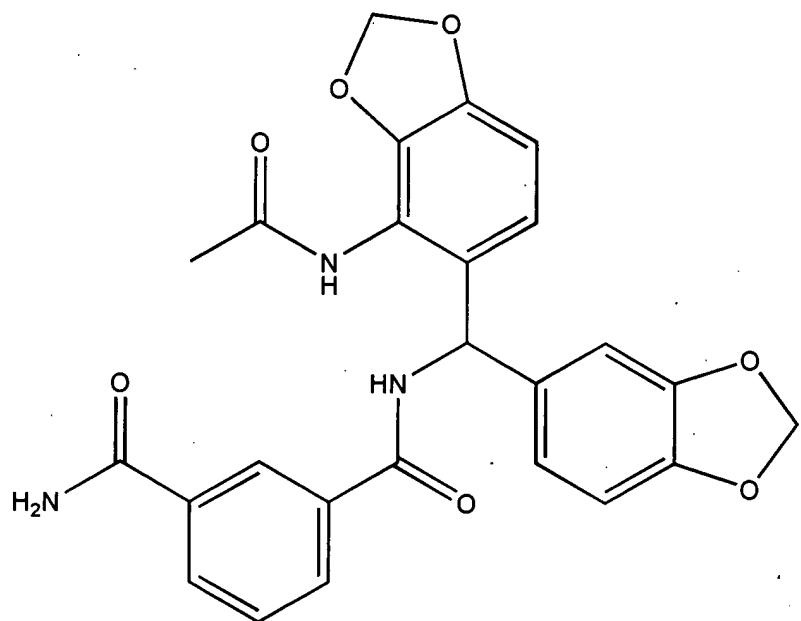
1:CLASS 2:Atom 3:Atom 4:Atom 5:CLASS 6:Atom 7:Atom 8:Atom 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom
30:Atom 31:Atom



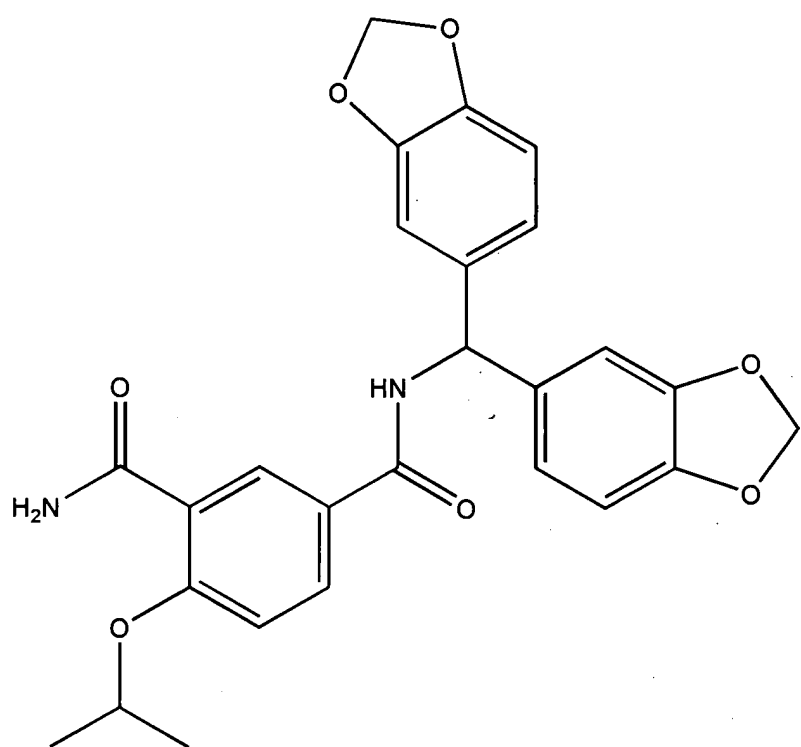
isophthalic acid di-(2,1,3-benzothiadiazol-5-yl) methyl ester



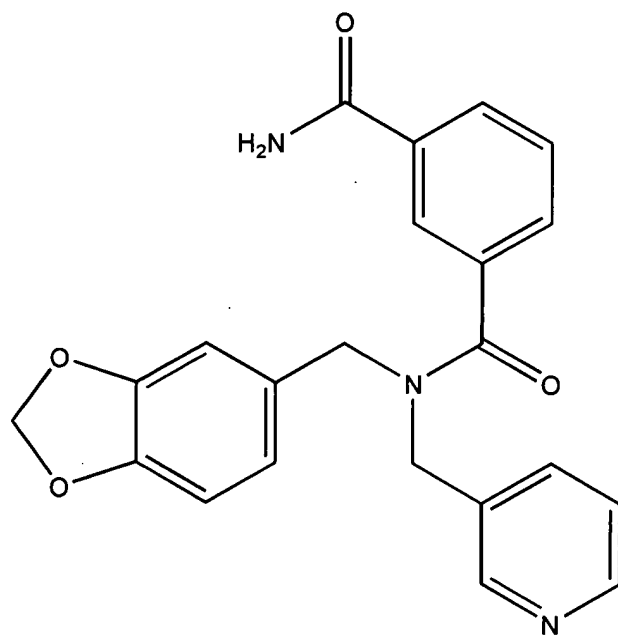
4-amino-bis-1,3-benzodioxol-5-ylmethyl-isophthalamide



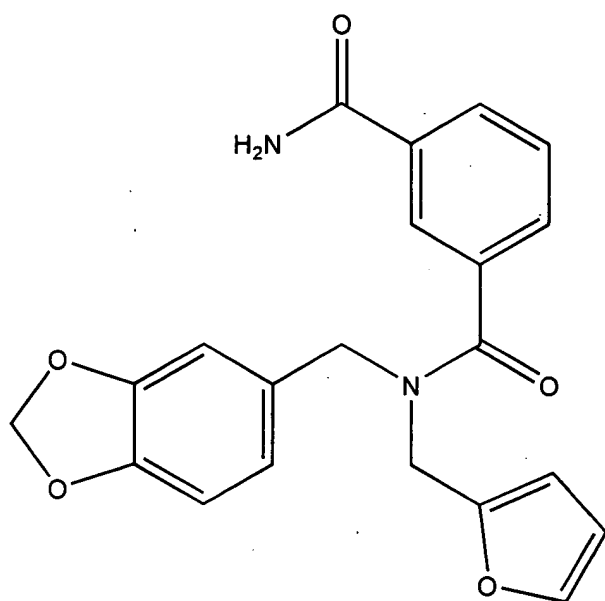
4-acetylamino-bis-1,3-benzodioxol-5-ylmethyl-isophthalamide



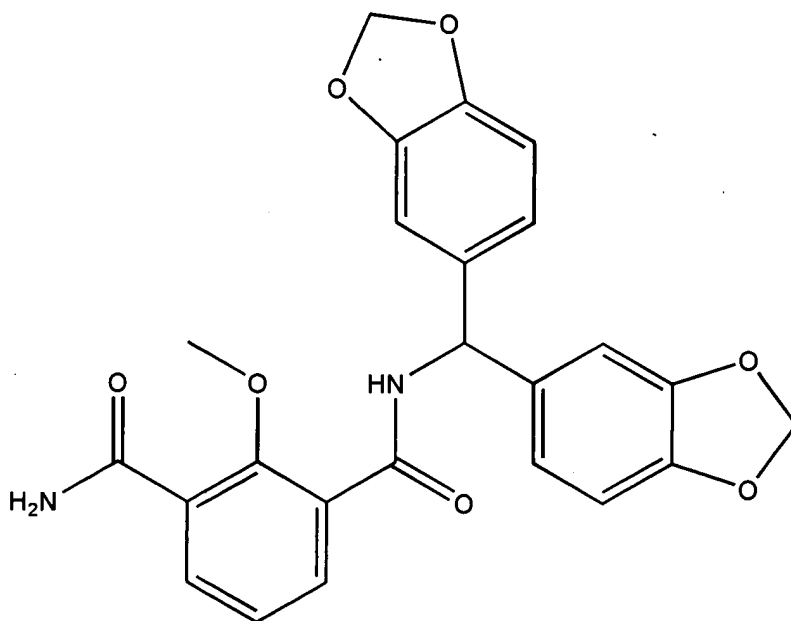
bis-1,3-benzodioxol-5-ylmethyl-4-isopropoxy-isophthalamide



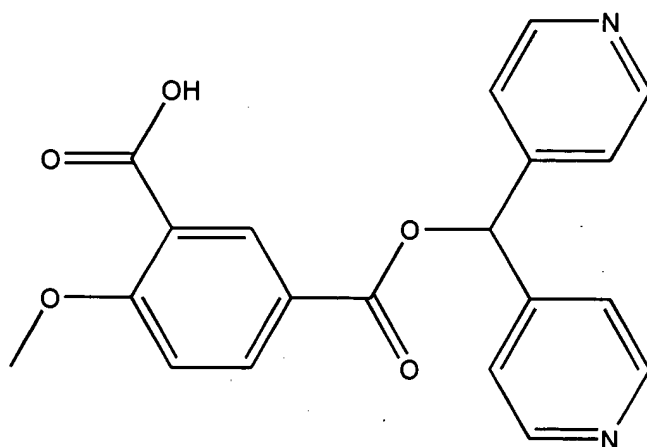
1,3-benzodioxol-5-ylmethyl-pyridin-3-ylmethyl-isophthalamide



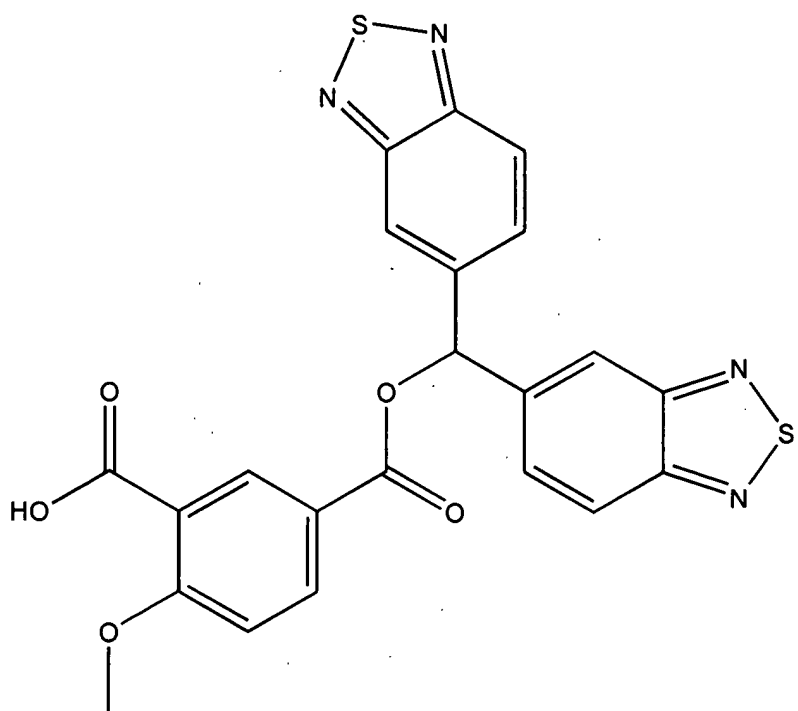
1,3-benzodioxol-5-ylmethyl-furan-2-ylmethyl-isophthalamide



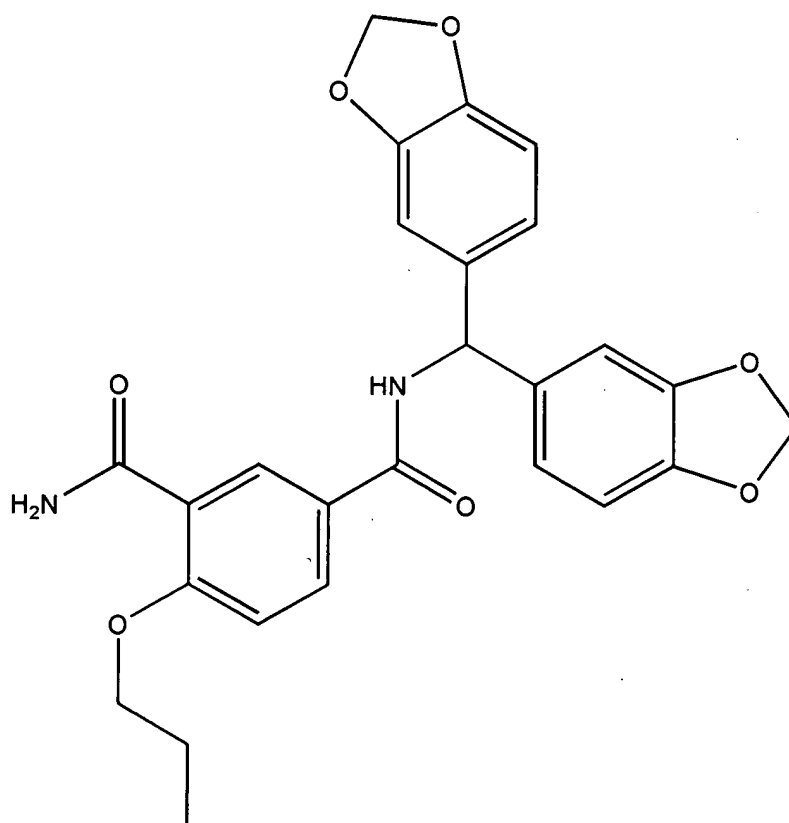
bis-1,3-benzodioxol-5-ylmethyl-methoxy-isophthalamide



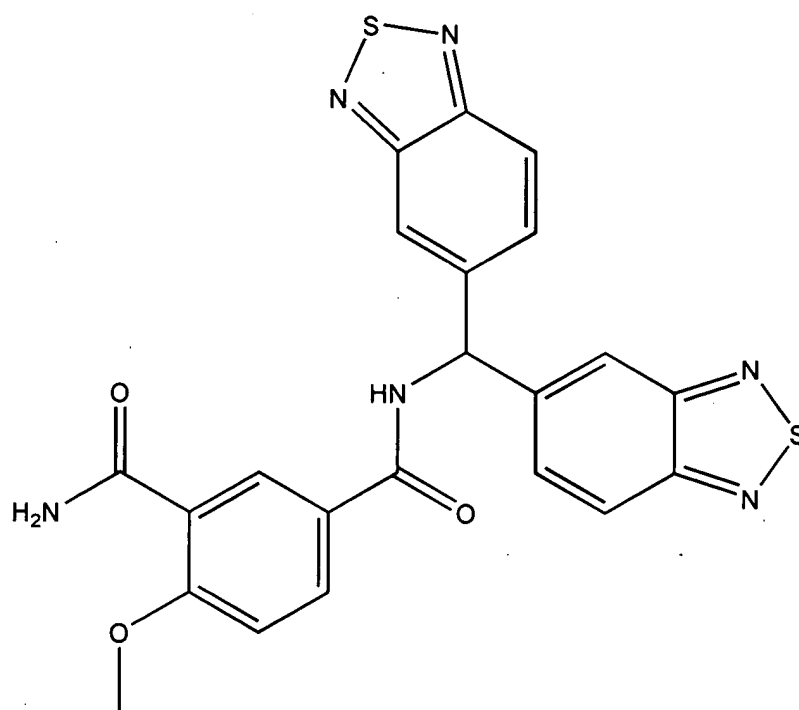
4-methoxy-isophthalic acid dipyridin-4-ylmethyl ester



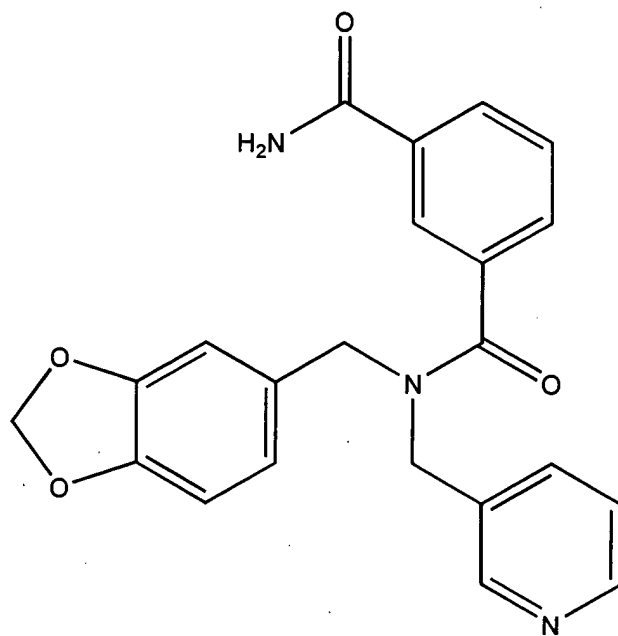
4-methoxy-isophthalic acid di-2,1,3-benzothiadiazol-5-ylmethyl ester



bis-1,3-benzodioxol-5-ylmethyl-4-propoxy-isophthalamide



bis-2,1,3-benzothiadiazol-5-ylmethyl-4-methoxy-isophthalamide



1,3-benzodioxol-5-ylmethyl-pyridin-3-ylmethyl-isophthalamide

Uploading C:\Program Files\Stnexp\Queries\918d.str

L17 STRUCTURE UPLOADED

=> d

L17 HAS NO ANSWERS

L17 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s 17

L18 636092 17

=> s 117

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 15:59:37 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 16 TO ITERATE

100.0% PROCESSED 16 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
PROJECTED ITERATIONS: 80 TO 560
PROJECTED ANSWERS: 0 TO 0

L19 0 SEA SSS SAM L17

L20 0 L19

=> s 117 full

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 15:59:43 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 361 TO ITERATE

100.0% PROCESSED 361 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L21 0 SEA SSS FUL L17

L22 0 L21

str

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l1

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 15:47:21 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 16 TO ITERATE

100.0% PROCESSED 16 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
PROJECTED ITERATIONS: 80 TO 560
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

L3 0 L2

=> s l1 full

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 15:47:27 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 361 TO ITERATE

100.0% PROCESSED 361 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L4 0 SEA SSS FUL L1

L5 0 L4

=>

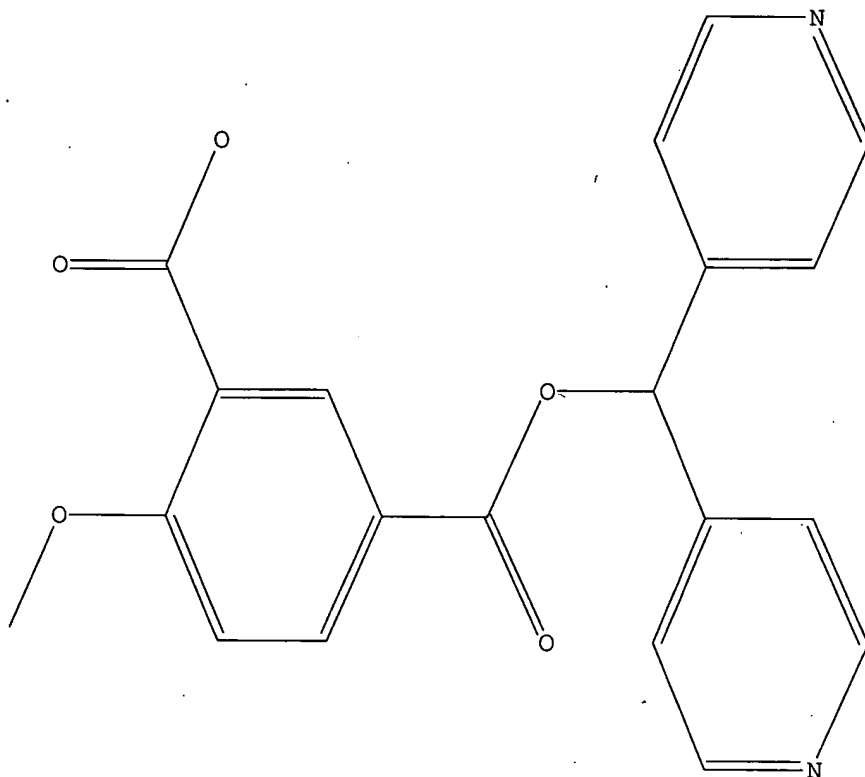
Uploading C:\Program Files\Stnexp\Queries\918-b.str

L6 STRUCTURE UPLOADED

=> d 16

L6 HAS NO ANSWERS

L6 STR



Structure attributes must be viewed using STN Express query preparation.

=> d 11

L1 HAS NO ANSWERS

L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s 16

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 15:49:39 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1287 TO ITERATE

77.7% PROCESSED 1000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 23588 TO 27892
PROJECTED ANSWERS: 0 TO 0

L7 0 SEA SSS SAM L6

L8 0 L7

=> s l6 full

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 15:49:46 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 26222 TO ITERATE

100.0% PROCESSED 26222 ITERATIONS
SEARCH TIME: 00.00.01

0 ANSWERS

L9 0 SEA SSS FUL L6

L10 0 L9

=>

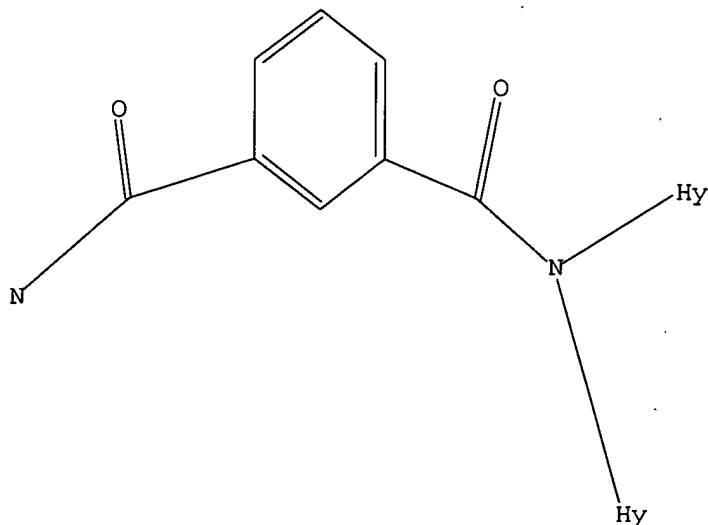
Uploading C:\Program Files\Stnexp\Queries\918c.str

L11 STRUCTURE UPLOADED

=> d

L11 HAS NO ANSWERS

L11 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l11

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 15:54:14 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 3453 TO ITERATE

29.0% PROCESSED 1000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 65536 TO 72584
PROJECTED ANSWERS: 0 TO 0

L12 0 SEA SSS SAM L11

L13 0 L12

=> s l11 full

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 15:54:20 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 68618 TO ITERATE

100.0% PROCESSED 68618 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

L14 2 SEA SSS FUL L11

L15 2 L14

=> s l15 and py<2001

20649979 PY<2001

L16 0 L15 AND PY<2001

=> d l15 1-2 ibib abs hitstr

L15 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:263059 CAPLUS
DOCUMENT NUMBER: 139:110540
TITLE: Dinuclear copper(II) complexes with different bridging
connectors
AUTHOR(S): Huang, W.; Hu, D.; Gou, S.; Qian, H.; Fun, H.-K.; Raj,
S. S. S.; Meng, Q.

CORPORATE SOURCE: State Key Laboratory of Coordination Chemistry,
Nanjing University, Nanjing, 210093, Peop. Rep. China
SOURCE: Journal of Molecular Structure (2003), 649(3), 269-278
CODEN: JMOSB4; ISSN: 0022-2860
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:110540

AB One novel triply-bridged dicopper(II) complex formulated as
[Cu₂(dpa)₂(μ-Cl)(μ-OH)(μ-HCOO)]·(ClO₄) (1, dpa =
2,2'-dipyridylamine) and two terephthalate anion bridged 2,2'-bipyridine
(2,2'-bpy) dicopper(II) complexes of [Cu₂(2,2'-bpy)₄(μ-
terephthalate)]·(NO₃)₂ (2) and [Cu₂(2,2'-bpy)₄(μ-
terephthalate)]·(terephthalate) (3), resp., were synthesized and
characterized by IR and electrospray mass spectra as well as x-ray
single-crystal determination Thermal properties of all compds. were studied.

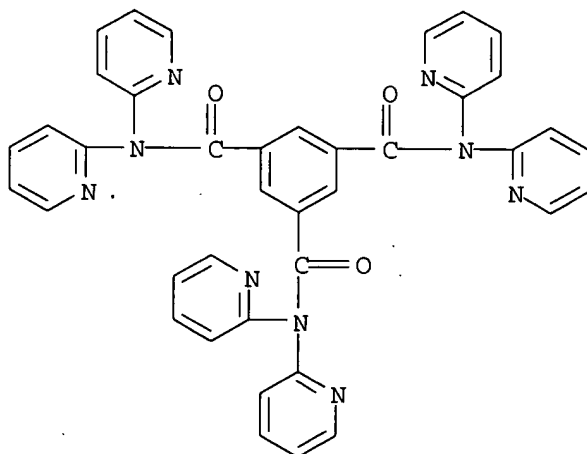
IT 557767-01-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(reactant for preparation of copper(II) chloro hydroxo formato
triply-bridged dipyrindylamine dinuclear complex)

RN 557767-01-8 CAPLUS

CN 1,3,5-Benzenetricarboxamide, N,N,N',N',N'',N''-hexa-2-pyridinyl- (9CI)
(CA INDEX NAME)



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:146239 CAPLUS

DOCUMENT NUMBER: 136:334309

TITLE: Synthesis and molecular structure of
N,N'-bis(2,2'-dipyridyl)isophthaloylamide as well as
its reaction with copper(II) perchlorate

AUTHOR(S): Hu, Dahua; Huang, Wei; Gou, Shaohua; Chantrapromma,
Suchada; Fun, Hoong-Kun; Xu, Yan

CORPORATE SOURCE: State Key Laboratory of Coordination Chemistry,
Nanjing University, Nanjing, 210093, Peop. Rep. China

SOURCE: Synthesis and Reactivity in Inorganic and
Metal-Organic Chemistry (2002), 32(1), 127-141
CODEN: SRIMCN; ISSN: 0094-5714

PUBLISHER: Marcel Dekker, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 136:334309

AB N,N'-Bis(2,2'-dipyridyl)isophthaloylamide (1) and its coordination product with a copper(II) ion, bis(2,2'-dipyridylamine)copper(II) diperchlorate (2), were prepared and spectroscopically characterized. X-ray structural results indicate that 1 has the expected configuration derived from the reaction between isophthaloyl dichloride and 2,2'-dipyridylamine (dpa) at a ratio of 1:2; while in complex 2, the copper atom is only coordinated to two dpa groups rather than the ligand 1 as anticipated. This known complex has a distorted tetrahedral configuration with two pyridine rings of each dpa moiety nearly coplanar to each other, and the dihedral angle of the two coordinating dpa ligands is 56.8°. Also the crystal structural study revealed that two-dimensional networks are formed by weak H-bonding interactions and π - π stacking interactions in both 1 and 2.

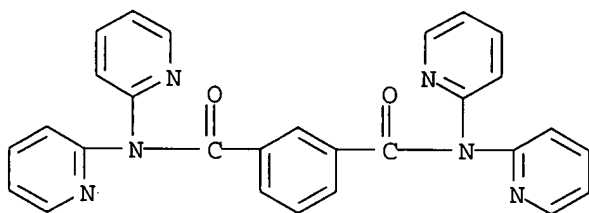
IT 325823-56-1P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and crystal and mol. structure and reaction with copper(II) perchlorate to give dipyridylamine complex)

RN 325823-56-1 CAPLUS

CN 1,3-Benzenedicarboxamide, N,N,N',N'-tetra-2-pyridinyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

13

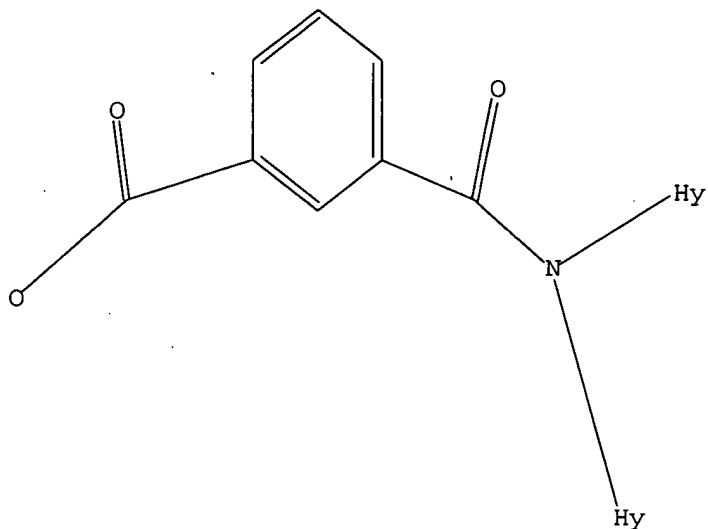
THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 STRUCTURE UPLOADED

=> d

L23 HAS NO ANSWERS

L23 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 123

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 16:04:20 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 9567 TO ITERATE

10.5% PROCESSED 1000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
PROJECTED ITERATIONS: 185479 TO 197201
PROJECTED ANSWERS: 0 TO 0

L24 0 SEA SSS SAM L23

L25 0 L24

=> s 123 full

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 16:04:27 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 191427 TO ITERATE

100.0% PROCESSED 191427 ITERATIONS
SEARCH TIME: 00.00.03

0 ANSWERS

L26 0 SEA SSS FUL L23

L27 0 L26

=>